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14. ABSTRACT

Numerical methods and a computer code have been developed for the simulation of multimaterial interactions in a general setting. Applications of concern to the Air Force include impact and penetration of targets, hazard prevention in the case of accidental impact on energetic materials, agent defeat, control of atmospheric spreading of hazardous multiphase material following impact etc. The equations governing material deformation and flow are solved in an Eulerian setting on a fixed Cartesian mesh. High-accuracy shock capturing schemes are applied to compute the nonlinear wave-propagation phenomena. Complex boundaries are tracked and their interactions are simulated using level-sets. Large deformations under high strain-rate conditions and multimaterial and multiphase interactions can be handled. The computer code has been parallelized and local mesh refinement techniques have been implemented to better resolve flow features.

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FINAL REPORT

PREDICTION AND ANALYSIS OF MATERIAL RESPONSE TO IMPACT AND SHOCK LOADING USING A SHARP-INTERFACE EULERIAN METHODOLOGY

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1. Introduction

We have developed numerical methods [1-4] and a computer code for the simulation of multimaterial interactions that result from high-speed munition impact. This is an important application with regard to the Air Force with implications for impact and penetration of targets, hazard prevention in the case of accidental impact on explosives, agent defeat, control of collateral damage, control of atmospheric spreading of hazardous material following impact etc. The direct beneficiary agency for this work is the AFRL-MNAC at Eglin AFB, FL. This work was initiated with encouragement from Dr. Kirk Vanden, chief of the Computational Mechanics Branch at AFRL-MNAC.

Any methodology to simulate material response to impact and shock loading should be able to handle the following physical phenomena:

1. Large deformations, including fragmentation and merger of the materials.
2. Nonlinear wave-propagation and the development of shocks in materials governed by rate-dependent plasticity.
3. Accurate elasto-plastic deformation of the interacting objects during impact.

A fixed-grid methodology carries the advantage of allowing for arbitrary deformation while avoiding problems associated with moving meshes. This implies that all moving bodies will be embedded in a fixed mesh and they will have to be tracked through the underlying mesh. Simultaneously, the dynamics of such moving bodies, i.e. deformation, collisions, break-ups etc. will have to be computed. A judicious choice of methodology to solve the governing equations as well as for tracking the moving boundaries has to be devised with high accuracy and robustness. The characteristics of the present numerical method that make it attractive relative to other methods employed in hydrocodes for high-speed multimaterial flows are:

1. The equations governing the material deformation are solved in an Eulerian setting on a fixed Cartesian mesh. Well-developed high-accuracy shock capturing schemes are easily applied to compute the nonlinear wave-propagation phenomena in this framework. Here the ENO scheme is used for all calculations. Addition of problem-dependent shock viscosity is not called for since adequate dissipation at discontinuities is built into the scheme.
2. The mesh remains fixed while the material flows through the mesh. Thus, issues such as mesh deformation, entangling, catastrophic mesh distortion in regions that have changed phase from solid to liquid and thus have lost strength, do not arise within the current fixed-grid approach. The materials can fragment or collide and/or merge without affecting the flow calculations.

3. The interfaces are tracked in a sharp fashion. They are not smeared over the mesh as in traditional Eulerian methods. Thus materials can approach each other without mixing and a mixture formulation is not required in treating cells with multiple interfaces or in cells that are only partially filled. The exact interface location is known at all times due to the level set representation. Boundary conditions and jump conditions can be applied at the sharp interfaces at both free surfaces and material-material interfaces.
4. A particle-level set method is used. This technique is shown to maintain sharp corners of objects without excessive smoothing due to the inherent entropy fix in the advection scheme used to evolve the narrow-band grid-based level set. Thus, spurious mass loss effects due to stretching and shearing of interfaces that plague all Eulerian interface tracking schemes are avoided in the present method. No difficulty arises in treating multiple boundaries. These are simply evolved as different level set functions. The interfaces can undergo topological changes without occasioning difficulties for the flow solver.
5. Extension to 3-dimensions is straightforward. The numerical schemes for the governing equations are obtained by field-by-field decomposition along each dimension and therefore addition of the third dimension will only necessitate discretization of the equations in that direction. Furthermore, the level set formulation is also easily extended to 3D, thus allowing for tracking of three-dimensional objects as a straightforward extension of the technique presented in this work.

2. Objectives and Significance

The overall project goals are as follows:

1. Advance the computational techniques for simulation of high-speed impact on fixed Cartesian meshes in several aspects, viz.:

(i) <u>Develop a local refinement strategy to improve the accuracy and efficiency of the method.</u> Cartesian methods suffer from lack of flexibility in placing grid points in locally refined regions. Thus, when the mesh needs to be refined to improve accuracy or capture small-scale features, the grid density increases globally. To overcome this drawback, local refinement techniques are being developed.

(ii) <u>Implement damage and materials models to be able to simulate material perforation and fragmentation.</u> Rate-dependent constitutive modeling such as in the Johnson-Cook model to model visco-plastic deformation has been implemented.

(iii) <u>Extend the method to 3-dimensions.</u> This is relatively straightforward to do within the framework of level-set-based interface representation. To render 3D simulations feasible parallelization of the code is imperative. The code is currently operational in parallel mode and further refinements are being performed to optimize performance.

2. Apply the method to problems of interest to collaborators at AFRL-MNAC (Eglin AFB, FL). The specific types of problems to be investigated include:

(i) The perforation and damage of metals under high strain-rate conditions, such as under the effects of shock loading, impact and detonation wave loading. Of particular interest are the micro-scale damage mechanisms, including void formation, growth and coalescence leading to spall in ductile materials.

(ii) Collapse of voids in energetic materials due to imposition of impact/shock loading. This problem is of interest in high-energy density explosives where accidental impact can initiate detonation and catastrophic explosion.

3. Work accomplished in this project

3.1 Simulations of high-speed multimaterial Interactions

For 2-dimensional problems the hybrid particle level set method has been used to track boundaries with sharp corners that are carried without deterioration through the large deformations of the materials. The details of the method have been presented in two journal papers [1-2]. Benchmark calculations for the multi-dimensional case including axisymmetric Taylor bar impact and penetration of a Tungsten rod into steel plate have shown excellent agreement with moving finite element solutions. Qualitative agreement with theory is shown for void collapsing process in an impacted material containing a spherical void. The method has thus been shown to be suitable for applications involving high-velocity, multimaterial impacts leading to large strain-rates, nonlinear elasto-plastic waves and topological changes.

An example of the capability [2] of the method is shown in Figure 1. The validation of our method for two deformable objects with different material properties (a case requiring 2 different level sets) is carried out using a slender tungsten heavy alloy (WHA) rod projectile penetrating an initially planar target made of a steel plate with a velocity of 1250 m/s. A Johnson-Cook material model is used and the corresponding strength parameters for both materials. Note that friction between the two impacting surfaces is neglected in these calculations. The evolution of equivalent plastic strain is shown in Figs. 1(a-c) for the extended domain with a 160x688 mesh. The maximum equivalent plastic strain is found to be around 4.5, occurring mostly near the impact surfaces. The values of equivalent plastic strain are higher in the WHA material compared to those in the steel material. The plastic strains obtained by Camacho and Ortiz [7] using Lagrangian finite element method with an adaptive mesh agree very well with the present results, both in terms of the magnitude and distributions of the plastic strains. In particular, a trough in the plastic strain distribution is noticed in both our results as well as those of Camacho and Ortiz and occurs near the bottom surface in the steel plate at the symmetry axis, as seen in Fig. 1(b). The ejection length of the WHA material is higher in the Camacho and Ortiz calculations when compared to our results. However, the resolution of the ejected region afforded by the mesh used in the present calculations is too low, with just 3 mesh points across the vertically oriented trails of the ejecta. The grid refinement study performed above indicates that as the mesh is refined further the length of the ejecta will increase. As shown below, at the current mesh resolution, the overall penetration characteristics and material deformation are adequately predicted. Fig. 2 shows the projectile nose and tail trajectories as a function of time, for the extended domain case, and is compared with the superposed results from experimental data and from Camacho and Ortiz [7]. Also plotted are the original rear and impact surfaces. Our results show reasonable agreement with those of experiment and Camacho and Ortiz. The tail trajectory is in much better agreement as its surface experiences less extreme conditions during impact and penetration. The present calculation predicts the penetration depth in good agreement with experiments. Despite the marginal resolution of the ejected trails, the overall penetration and deformation behavior is predicted in good accord with the adaptive finite element simulations of Camacho and Ortiz.

3.2 Investigation of thermomechanics of void collapse in an energetic material

In the recently completed PhD work of Linhbao Tran, the methodology was advanced to include the thermomechanics of void collapse in an energetic material that is subject to shock loading. The Eulerian, *sharp interface*, fixed Cartesian grid method was applied to study hot spot formation in an energetic material (HMX) under various loading conditions [3-4]. The mass, momentum, and energy equations were solved along with evolution equations for deviatoric stresses and equivalent plastic strain. These equations were cast in Eulerian conservation law form. Pressure was obtained from the Mie-Grüneisen equation of state. The material was modeled as a viscoplastic solid. High-order accurate ENO shock-capturing schemes along with a particle level set technique were used to evolve sharp immersed boundaries. The details of void collapse under shock-loading and the coupling of the void dynamics to the energy release in the solid material were analyzed and are presented in the papers [3-4]. The thermo-mechanical response of solid phase was combined with the vapor-phase compression and chemical reactions to study their effects on the energy deposition mechanisms. The formulation and numerical treatment of the coupled solid-gas interactions, including heat release due to chemical reactions was also successfully tackled. The effects of loading intensity and void size were studied. The results show that for the micron-size voids under consideration significant gas phase chemical reactions occur. However, their influence on the void collapse itself is minimal. Figure 3 shows a sample result for the collapse of a 20 micron diameter void when the lower boundary of the domain is subject to shock loading with imposed particle velocity of U_p=100m/s. When the shock collapses there is a hot spot created where significant chemical reactions occur leading to the breakdown of HMX into monomer and other reactive components. The point of collapse is also a region of high temperature and pressure and a compression wave emanates from the collapse point to the surrounding material. Results [3-4] indicate that for micron-size voids the collapse time is too short to set up thermal runaway at the hot spot prior to void collapse.

3.3 Extension to multimaterial interactions in low-speed flows

As an extension of the method development research that is being undertaken in this project, advances have resulted in the development of the level-set-based technique for handling of low-speed (incompressible flow regime) fluid-solid interaction problems. The attractive feature of the current research is the generality that it affords in handling a wide range of multimaterial problems with moving boundaries in 3-dimensions. In recently submitted papers [5-6] we have demonstrated the capability of the method to tackle fluid-structure interaction problems [5] and droplet-surface interaction problems [6]. In these papers the ease of implementation of the technique in 3-dimensions for such problems has also been demonstrated. These applications were made possible by the general idea of using level-sets to track boundaries and the ability to handle collisions of interfaces. The central theme of the current research effort, i.e. to develop a sharp-interface discretization strategy has been used in these papers. Validation of the numerical results has been performed in each case with experimental data and other numerical/analytical solutions.

A fluid-structure interaction problem, that of a sphere oscillating in a stratified fluid, is shown as an example in Figure 4. For a specific set of sphere oscillation frequency and Reynolds number of the oncoming flow, the vortical structures visualized using the Δ-method are plotted in Figure 4. The cylindrical vortices apparent in the x-y view shown in Figure 4(b) illustrate that the vortex shedding is self similar in z-direction. This demonstrates the quasi-two-dimensionality imposed due to stratification and is in perfect agreement with the experiments on this problem [8]. The x-z view of vortex shedding shown in Figure 4(c) supports the above observation. The Strouhal number

calculated from the probe velocity variation with time is 0.35 which indicates that the shedding under these conditions locks on with the oscillation frequency of the sphere. Figure 4 also illustrates that the vortices are being shed alternately from either side of the sphere. Hence this flow regime is named "lock-on alternate single vortex" regime [8]. The flow structures viewed from the various perspectives are visually identical to those obtained in the experiments [8]. In summary, flow around an oscillating sphere in the presence of density stratification has been simulated for a selected set of parameters. The flow regimes, vortical patterns and shedding frequencies predicted by the current technique for these test points are in agreement with the experimental results reported by Lin & coworkers and thereby provide validation for the present methodology for three-dimensional incompressible flows involving moving immersed objects.

A sample result of multimaterial incompressible flows is shown in Figure 5 (see [6] for extensive validation of the method for such applications). The calculation carried out is for a water droplet suspended in air which falls on a stationary solid cylindrical surface. The following dimensionless parameters apply: Reynolds number Re=10, Weber number We=10, and Froude number Fr=1. The liquid droplet (density of the liquid is 100 times that of the surrounding air) starts to move down due to gravity, impacts on the curved surface, spreads and drips down, as observed in Figure 5. Eventually, this droplet undergoes severe deformation following which the droplet breaks and forms two smaller drops that fall under gravity. The falling film of fluid then retracts due to capillary forces and accumulates to form a second drop, which in turn is pulled down due to gravity and breaks away from the main drop. This problem shows the capability of the method to track interactions and severe deformations of boundaries in low-speed flows.

4. Work in Progress and extensions

The capability to compute the flows in 3D has been developed in the framework of a fixed Cartesian mesh and level-set representation of the interfaces. In order to make 3D computations feasible, the code has been parallelized using MPI (Message Passing Interface). Local mesh refinement using an octree structure to subdivide the mesh points has also incorporated into the code. The use of local mesh refinement produces issues that conflict with parallel efficiency and thus care needs to be exercised in coordinating the parallel implementation with mesh refinement strategy. Furthermore the behavior of waves at fine-coarse mesh interfaces needs to be carefully treated or spurious wave reflections or damping will result. These challenging issues are being addressed in current work.

5. References

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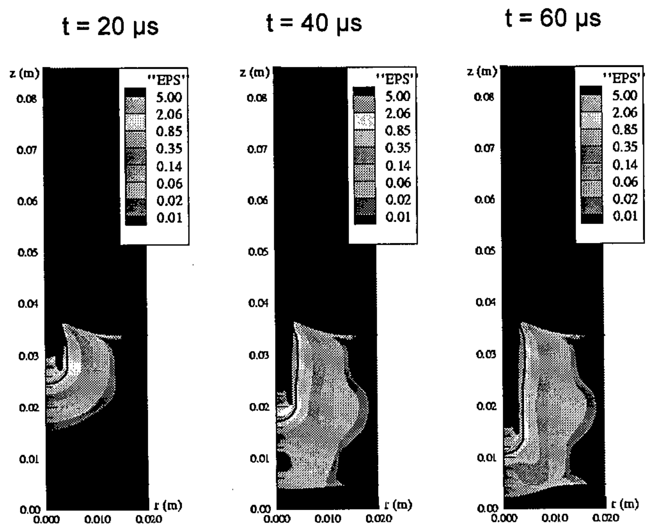

Figure 1. Simulation of penetration of a Tungsten rod into a steel plate. Impact velocity is 1.25 km/s. The shapes of the rod and plate are shown at three instants of time. Contours of plastic strain are also shown.

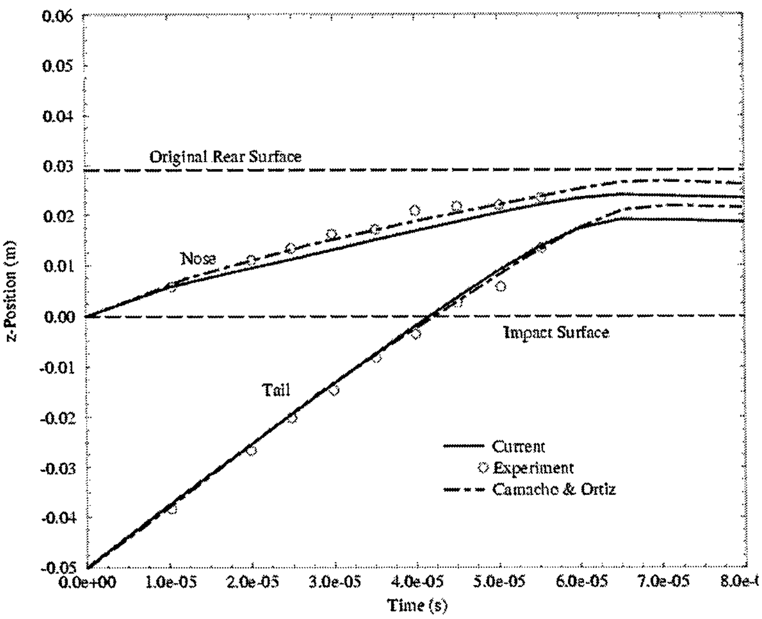

Figure 2. Comparison of the positions of the tail and head of the Tungsten rod shown in Figure 1 as obtained from the current calculation and the numerical (FEM) benchmark [8] and experimental data.

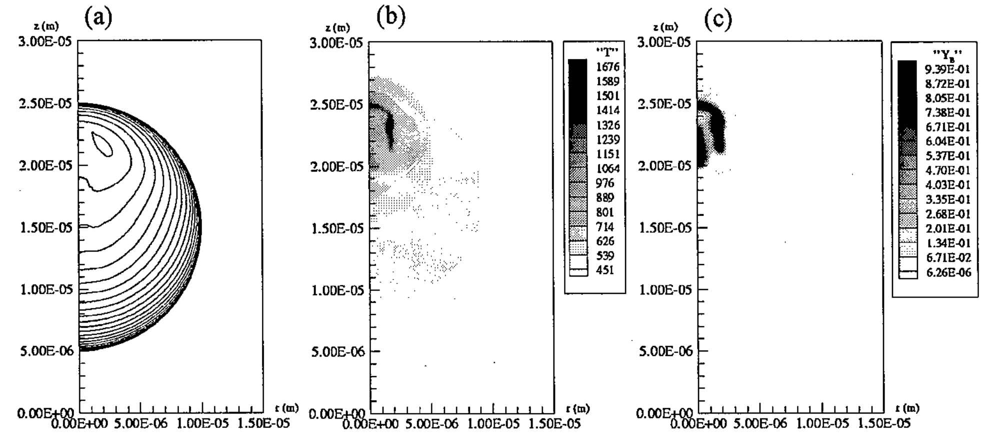

Figure 3. (a) Evolution of void collapse process for void diameter of 20 microns, impact velocity of 100 m/s imposed on the lower surface of the computational domain, shock rise time of 10 ns. (b) Temperature field at point of collapse. (c) Decomposed HMX species concentration field at point of void collapse.

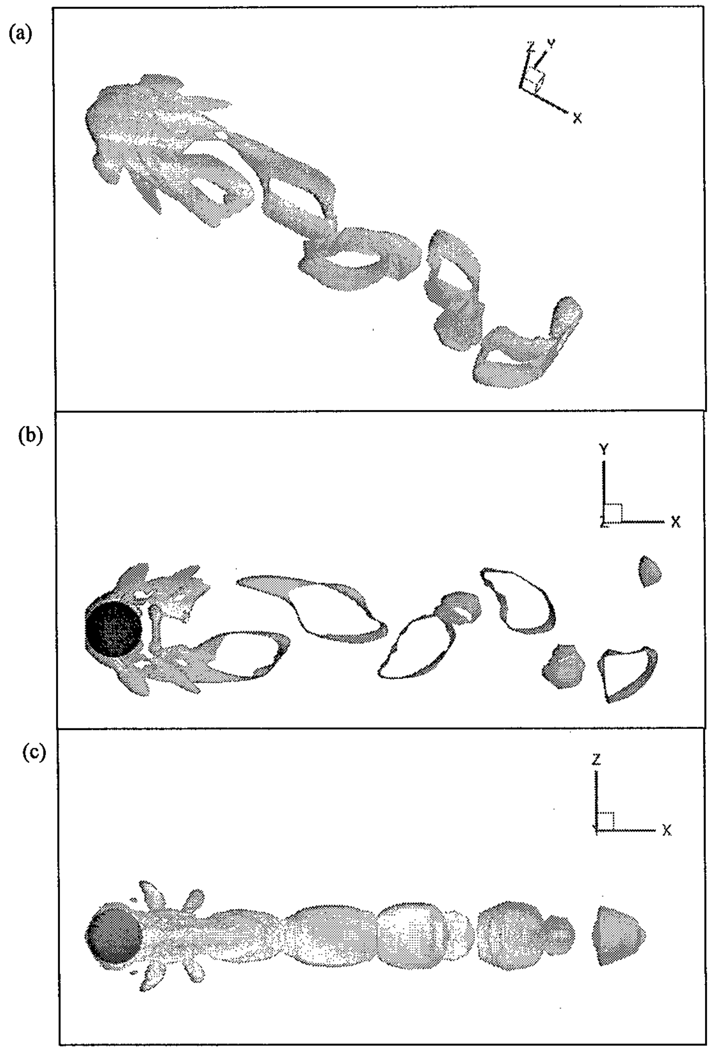

Figure 4. Results for 3-dimensional fluid-solid interaction problem. A sphere oscillates in the streamwise direction with an oncoming flow in a stratified fluid (stratification is along z-direction). The figures show vertical structures at a Reynolds number of 190 for a specific oscillation frequency of the sphere. See [3] for details. (a) Oblique view, (b) x-y view, (c) x-z view.

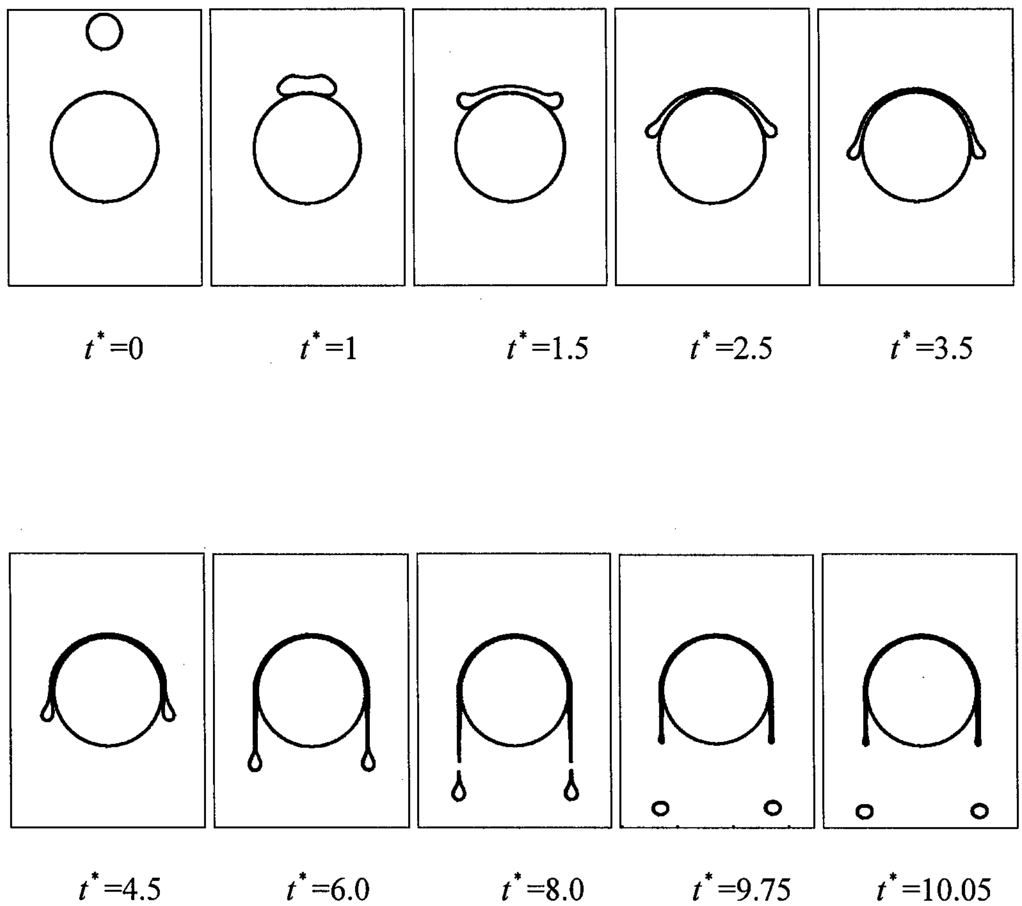

Figure 5. Shapes of a droplet impacting on a cylinder (Re=10, We=333). The formation of a filament on each side is seen along with the detachment of a pendant drop and formation of a secondary pendant drop after retraction of the remaining filament.